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L3            25 S L1 FULL

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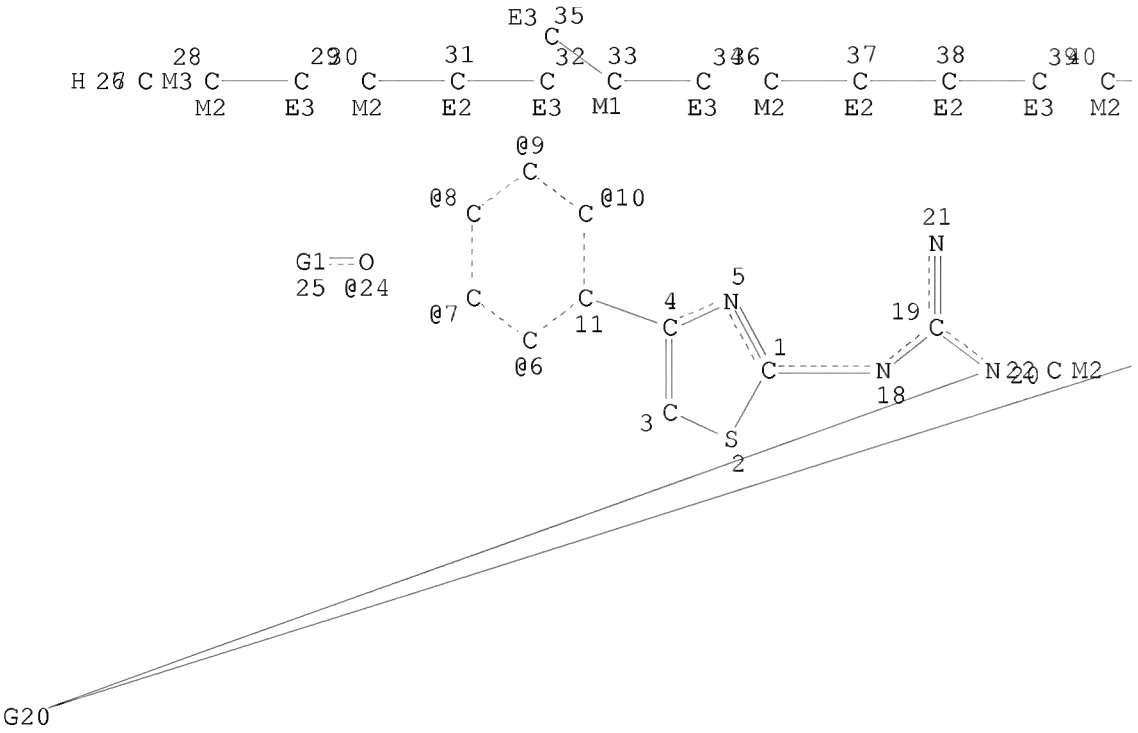

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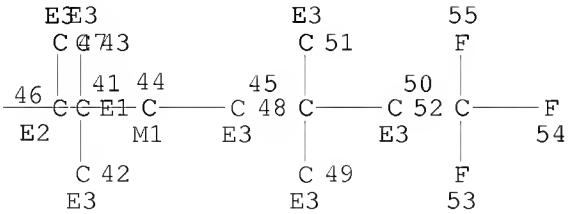

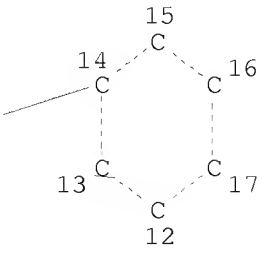

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GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  55

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED     224 ITERATIONS                          25 ANSWERS
SEARCH TIME: 00.00.01



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L5            2 L3 NOT L4

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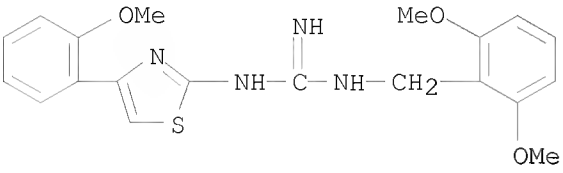
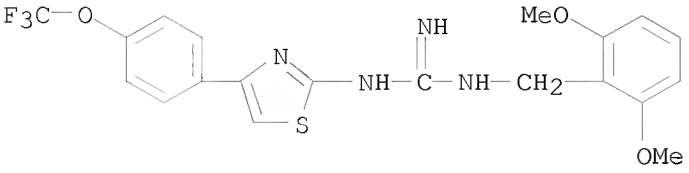
L5 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2011 ACS on STN
RN 863707-11-3 REGISTRY
ED Entered STN: 22 Sep 2005
CN Guanidine, N-[(2,6-dimethoxyphenyl)methyl]-N'-[4-(2-methoxyphenyl)-2-thiazolyl]- (CA INDEX NAME)
MF C20 H22 N4 O3 S
CI COM
SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2011 ACS on STN
RN 863707-01-1 REGISTRY
ED Entered STN: 22 Sep 2005
CN Guanidine, N-[(2,6-dimethoxyphenyl)methyl]-N'-[4-[4-(trifluoromethoxy)phenyl]-2-thiazolyl]- (9CI) (CA INDEX NAME)
MF C20 H19 F3 N4 O3 S
CI COM
SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2011 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 17 Sep 2011  VOL 155 ISS 13
FILE LAST UPDATED: 16 Sep 2011  (20110916/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Jun 2011
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Jun 2011

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2011.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.
'.FIONA' IS DEFAULT FORMAT FOR 'CAPLUS' FILE

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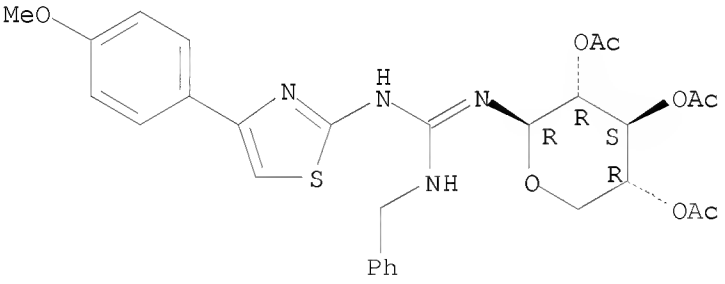
L6 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2007:1183783 CAPLUS
DOCUMENT NUMBER: 149:201128
TITLE: Synthesis of N-alkyl/aryl-N'-(4-aryl-2-thiazolyl)-N''-xylopyranosyl guanidines
AUTHOR(S): Li, Gen; Wu, Peng; Cao, Ling Hua
CORPORATE SOURCE: College of Chemistry and Chemical Engineering, Xinjiang University, Urumqi, 830046, Peop. Rep. China
SOURCE: Heteroatom Chemistry (2007), 18(6), 688-694
CODEN: HETCE8; ISSN: 1042-7163
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:201128
ABSTRACT:
A reaction of 2,3,4-tri-O-acetyl-β-D-xylopyranosyl isothiocyanate with 2-amino-4-(aryl)thiazole derivs. gave xylopyranosyl thiourea derivs. These thiourea derivs. reacted with alkyl amine or aryl amine derivs. in the presence of HgCl2 to give a new series of N-alkyl-N''-(4-aryl-2-thiazolyl)-N''-xylopyranosyl guanidine and N-aryl-N''-(4-aryl-2-thiazolyl)-N''-xylopyranosyl guanidine derivs. Some of these guanidines were screened for their biol. activity as HIV-1 protease inhibitors.

IT **1041178-31-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of N-alkyl-N'-[(phenyl)thiazolyl]-N''-(triacetyl-β-D-xylopyranosyl)guanidine and N-aryl-N'-[(phenyl)thiazolyl]-N''-(triacetyl-β-D-xylopyranosyl)guanidine derivs.)
RN 1041178-31-7 CAPLUS
CN Guanidine, N-[4-(4-methoxyphenyl)-2-thiazolyl]-N''-(phenylmethyl)-N'-(2,3,4-tri-O-acetyl-β-D-xylopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2005:959678 CAPLUS
DOCUMENT NUMBER: 143:266930
TITLE: Guanidine compounds and their use as ligands for 5HT receptors
INVENTOR(S): Netz, Astrid; Amberg, Wilhelm; Lange, Udo; Ochse, Michael; Kling, Andreas; Hutchins, Charles W.; Garcia-Ladona, Francisco-Xavier; Wernet, Wolfgang
PATENT ASSIGNEE(S): Abbott GmbH & Co. Kg, Germany
SOURCE: Ger. Offen., 52 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 102004008141	A1	20050901	DE 2004-102004008141	20040219
WO 2005082871	A2	20050909	WO 2005-EP1521	20050215
WO 2005082871	A3	20051110		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1716127	A2	20061102	EP 2005-707406	20050215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR, IS				
JP 2007523113	T	20070816	JP 2006-553516	20050215
JP 4658073	B2	20110323		
MX 2006009434	A	20070321	MX 2006-9434	20060818
US 20070299074	A1	20071227	US 2007-590265	20070614

PRIORITY APPLN. INFO.: DE 2004-102004008141A 20040219
WO 2005-EP1521 W 20050215
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 143:266930
GRAPHIC IMAGE:

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

ABSTRACT:
The present invention concerns guanidine compds., e.g., I [R1, R2, R3 = H, OH, CN, (un)substituted C1-6-alkyl, C1-4-alkoxy, C2-6-alkenyl, C3-12-alkynyl, CO-(C1-6-alkyl), CO2-(C1-6-alkyl), etc.; R4, R5 = H, halogen, CN, CF3, CHF2, C1-10-alkyl, Ph, naphthyl, heteroaryl, etc.; R4R5 = (un)substituted 4- to 7-membered ring, optionally containing addnl. O, S, N; Q = Q1, Q2, Q3, Q4, Q5, Q6; W = W1, W2; Z = (CRz1Rz2)a(V)b(CRz3Rz4)c; A, D = NO2, NH2, OH, CN, CF3, OCF3, CHF2, OCHF2, CO2H, OCH2CO2H, halogen, SH, etc.; B = H, A; R' = H, OH, halogen, NO2, NH2, CN, CF3, CHF2, OCF3, OCHF2, (un)substituted C1-6-alkyl,

C3-7-cycloaalkyl, (C1-6-alkene)-O-(C1-6-alkyl), C2-6-alkenyl, C3-12-alkynyl, CO-(C1-6-alkyl), CO2-(C1-6-alkyl), SO2-(C1-6-alkyl), etc.; a = 0 - 4; b = 0, 1; c = 0 - 4; Rz1, Rz2, Rz3, Rz4 = H, halogen, OH, etc.; E = O, NRq1, S; V = CO, CONR, NRCO, O, S, SO, SO2, SO2NR, NRSO2, CS, CSNR, NRCS, etc.; Rq1 = H, C1-4-alkyl, CO-(C1-4-alkyl),SO2-(C1-4-alkyl), CO2-(C1-4-alkyl), etc.] , their enantiomers, diastereomers and/or tautomeric forms as well as pharmaceutical acceptable salts thereof. Thus, N-(2-methoxybenxyl)-N'-(11,3-thiazol-2-ly)guanidine (II) was prepared from 2-aminothiazole via reaction with thiocarbonyldiimidazole in MeCN, ammonolysis with NH4OAc in EtOH, N-methylation in MeOH and amidation with 2-MeOC6H4CH2NH2 in EtOH. Further the present compound concerns the use of guanidine compds. as ligands for 5HT receptors for the treatment of diseases, which are modulated by a 5HT receptor activity, in particular for the treatment of neurodegenerative and neuropsychiatric disturbances as well as the signs, symptoms and malfunctions which are connected with it. The pharmacol. activity off II was determined [Ki = 50 nM].

IT **863657-14-1P** **863657-17-4P** **863657-20-9P**
863657-32-3P **863657-60-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(guanidine derivs. and their use as ligands for 5HT receptors)

RN 863657-14-1 CAPLUS
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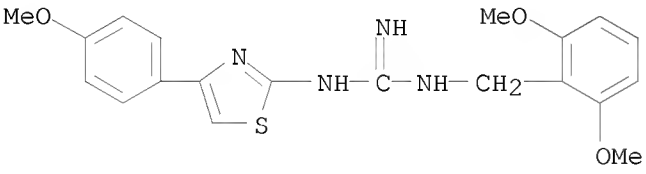

RN 863657-17-4 CAPLUS
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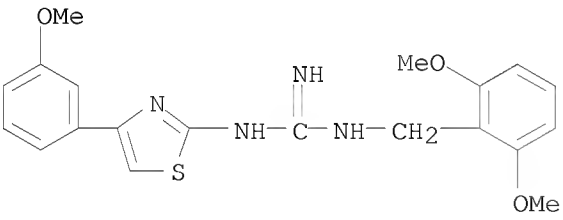

RN 863657-20-9 CAPLUS
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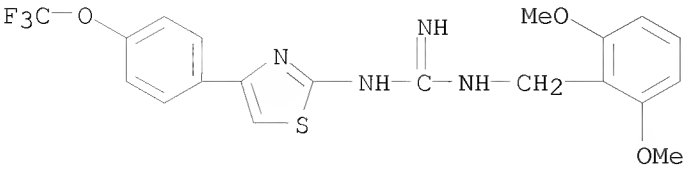

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RN 863657-32-3 CAPLUS
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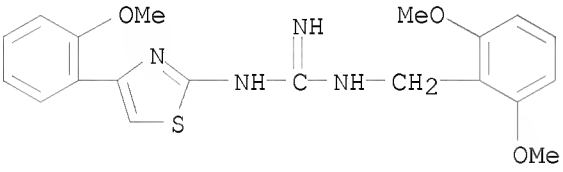
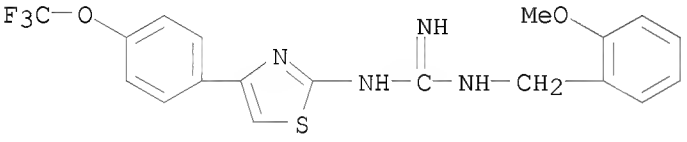


● HBr

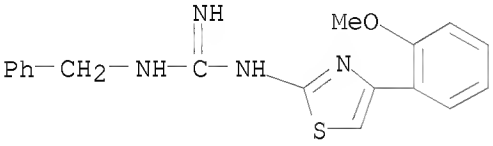
RN 863657-60-7 CAPLUS
CN Guanidine, N-[(2-methoxyphenyl)methyl]-N'-[4-[4-(trifluoromethoxy)phenyl]-2-thiazolyl]- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L6 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2001:173569 CAPLUS
DOCUMENT NUMBER: 135:55445
TITLE: QSAR study of anti-ulcer compounds using calculated parameters
AUTHOR(S): Grunheidt Borges, E.; Takahata, Y.
CORPORATE SOURCE: Instituto de Quimica, Universidade Estadual de Campinas, Campinas, Sao Paulo, 13081-970, Brazil
SOURCE: Journal of Molecular Structure: THEOCHEM (2001), 539, 245-251
CODEN: THEODJ; ISSN: 0166-1280
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
The biol. activity measured exptl. for a series of mols. was used to create a QSAR model using the parameters calculated with the semi-empirical method AM1 and the mol. vols. The statistical methods, such as partial least squares, pattern recognition techniques and principal component anal., were used to work with a large amount of data and establish QSAR. Cross-validation was used to test the predictive capability of the model. The anal. of the data allows one to draw some conclusions about the importance of some mol. parameters. The results can provide information about how to model better drugs.

IT **123309-99-9** **123310-00-9** **123310-07-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(QSAR study of antiulcer compds. using calculated parameters)
RN 123309-99-9 CAPLUS
CN Guanidine, N-[4-(2-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-00-9 CAPLUS
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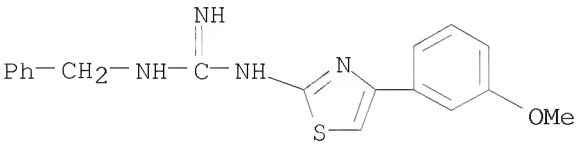
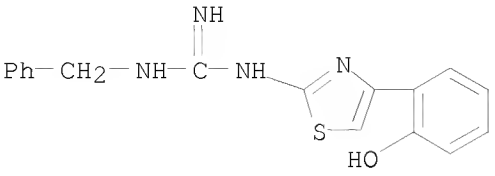
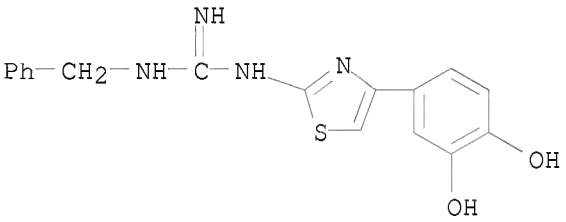


RN 123310-07-6 CAPLUS
CN Guanidine, N-[4-(2-hydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



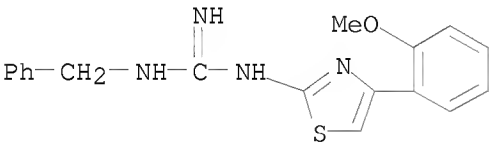
IT **123310-11-2**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(QSAR study of antiulcer compds. using calculated parameters)
RN 123310-11-2 CAPLUS
CN Guanidine, N-[4-(3,4-dihydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1999:683956 CAPLUS
DOCUMENT NUMBER: 132:117084
TITLE: Superpendentic Index: a novel topological descriptor for predicting biological activity. [Erratum to document cited in CA131:179]
AUTHOR(S): Gupta, S.; Singh, M.; Madan, A. K.
CORPORATE SOURCE: Dep. Pharmaceutical Sciences and Drug Research, Punjabi Univ., Patiala, 147 002, India
SOURCE: Journal of Chemical Information and Computer Sciences (1999), 39(6), 1230
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
The corrected equation for page 272 is given.

IT **123309-99-9** **123310-00-9** **123310-02-1**
123310-04-3 **123310-07-6** **123310-08-7**
123310-09-8 **123310-11-2** **123310-13-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(superpendentic index as a novel topol. descriptor for predicting biol. activity (Erratum))
RN 123309-99-9 CAPLUS
CN Guanidine, N-[4-(2-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



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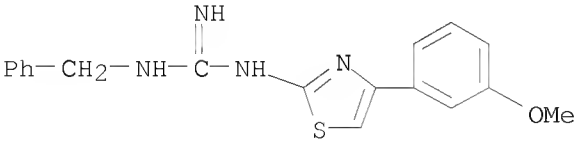

RN 123310-02-1 CAPLUS
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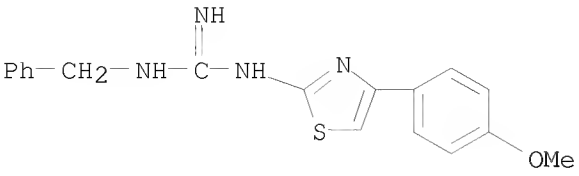

RN 123310-04-3 CAPLUS
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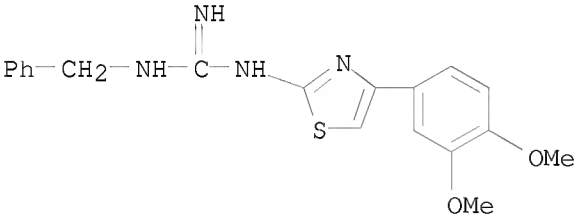
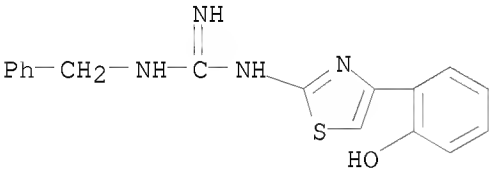
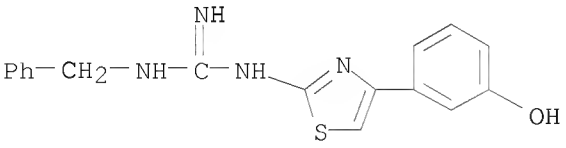


RN 123310-07-6 CAPLUS
CN Guanidine, N-[4-(2-hydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-08-7 CAPLUS
CN Guanidine, N-[4-(3-hydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-09-8 CAPLUS
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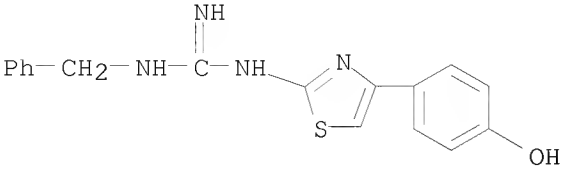
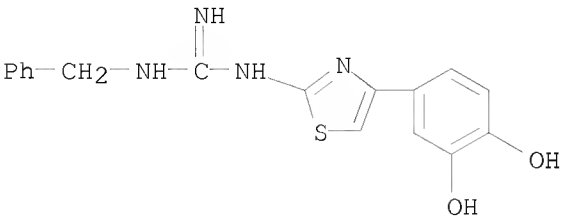
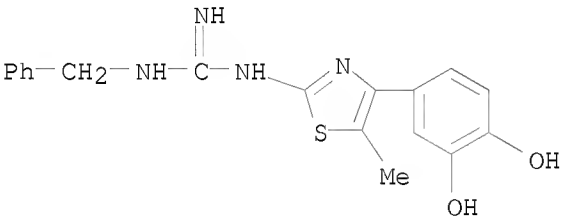


RN 123310-11-2 CAPLUS
CN Guanidine, N-[4-(3,4-dihydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-13-4 CAPLUS
CN Guanidine, N-[4-(3,4-dihydroxyphenyl)-5-methyl-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



L6 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1999:142811 CAPLUS
DOCUMENT NUMBER: 131:179
TITLE: Superpendentic Index: A novel topological descriptor for predicting biological activity
AUTHOR(S): Gupta, S.; Singh, M.; Madan, A. K.
CORPORATE SOURCE: Department of Pharmaceutical Sciences and Drug Research, Punjabi University, Patiala, 147 002, India
SOURCE: Journal of Chemical Information and Computer Sciences (1999), 39(2), 272-277
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
A simple highly degenerating, pendenticity based, topol. descriptor termed as superpendentic index has been conceptualized and its discriminating power investigated with regard to antiulcer activity. A data set consisting of 128 analogs of 4-substituted-2-guanidino thiazoles was selected for the present study. These analogs are reversible, competitive, and selective inhibitors of gastric H+,K+-ATPase enzyme. The value of superpendentic index of each analog in the data set was computed and active range was identified. The biol. activity assigned to each analog using superpendentic index was subsequently compared with the reported in vitro and in vivo inhibitory activities. The accuracy of classification of analogs based on in vivo activity was found to be 82% in the active range using superpendentic index.

IT **123309-99-9** **123310-00-9** **123310-02-1**
123310-04-3 **123310-07-6** **123310-08-7**
123310-09-8 **123310-11-2** **123310-13-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(superpendentic index as novel topol. descriptor for predicting biol. activity)

RN 123309-99-9 CAPLUS
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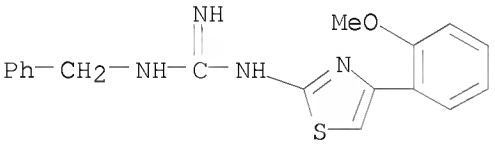

RN 123310-00-9 CAPLUS
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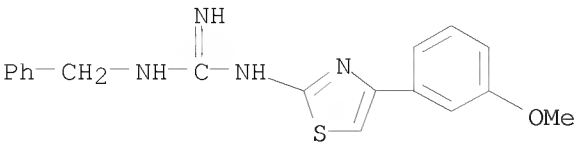
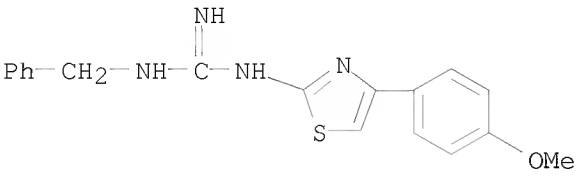


RN 123310-02-1 CAPLUS

CN Guanidine, N-[4-(4-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-04-3 CAPLUS
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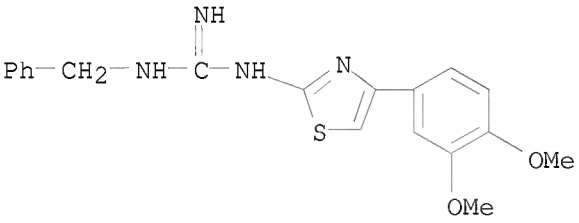

RN 123310-07-6 CAPLUS
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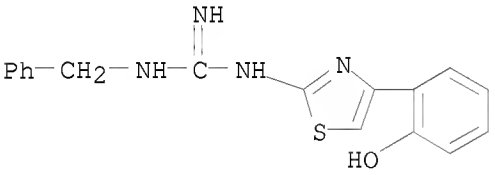
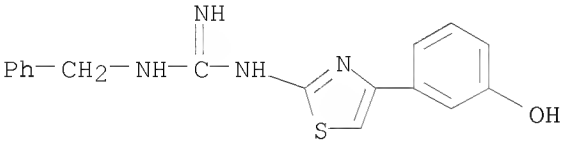
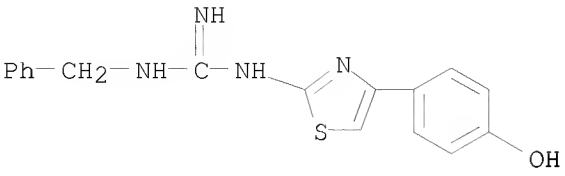


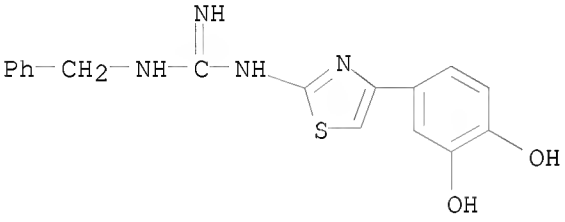
RN 123310-08-7 CAPLUS
CN Guanidine, N-[4-(3-hydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



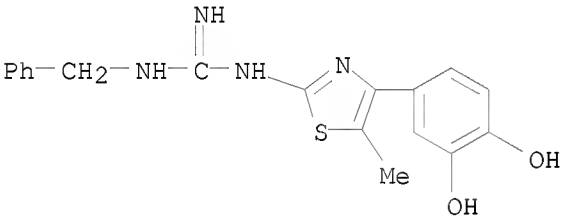
RN 123310-09-8 CAPLUS
CN Guanidine, N-[4-(4-hydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-11-2 CAPLUS
CN Guanidine, N-[4-(3,4-dihydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-13-4 CAPLUS
CN Guanidine, N-[4-(3,4-dihydroxyphenyl)-5-methyl-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)

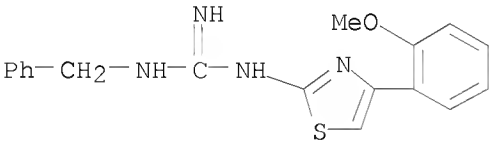


OS.CITING REF COUNT: 52 THERE ARE 52 CAPLUS RECORDS THAT CITE THIS RECORD (52 CITINGS)
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

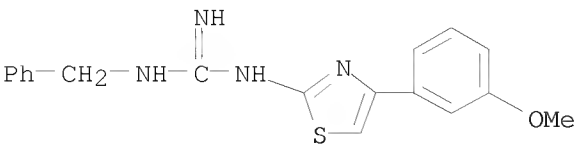
L6 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1995:568674 CAPLUS
DOCUMENT NUMBER: 122:281411
ORIGINAL REFERENCE NO.: 122:51019a,51022a
TITLE: Structure-Activity Study on Antiulcer Agents Using Wiener's Topological Index and Molecular Connectivity Index
AUTHOR(S): Goel, Anshu; Madan, A. K.
CORPORATE SOURCE: College of Pharmacy, Pushp Vihar, New Delhi, 110 017, India
SOURCE: Journal of Chemical Information and Computer Sciences (1995), 35(3), 504-9
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
The relation of Wiener's topol. index and mol. connectivity index with antiulcer activity of a series of 4-substituted-2-guanidino thiazole analogs has been investigated. The values of Wiener's topol. index and mol. connectivity index of 128 compds. were computed and active ranges were identified. The activity assigned to each analog using these topol. descriptors was subsequently compared with the reported in vitro and in vivo activities against gastric hydrogen-potassium stimulated ATPase (H+K+-ATPase) enzyme. Predictions with an accuracy of the order of .apprx.89% were observed with regard to in vivo activity using these topol. indexes.

IT **123309-99-9** **123310-00-9** **123310-02-1**
123310-04-3 **123310-07-6** **123310-08-7**
123310-09-8 **123310-11-2** **123310-13-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(structure-activity study on antiulcer guanidinothiazoles using Wiener's topol. index and mol. connectivity index)

RN 123309-99-9 CAPLUS
CN Guanidine, N-[4-(2-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)

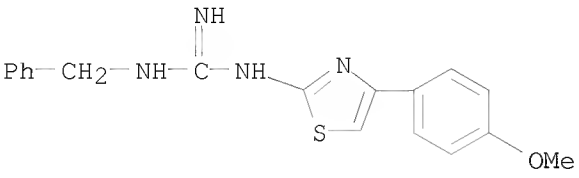


RN 123310-00-9 CAPLUS
CN Guanidine, N-[4-(3-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-02-1 CAPLUS

CN Guanidine, N-[4-(4-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-04-3 CAPLUS
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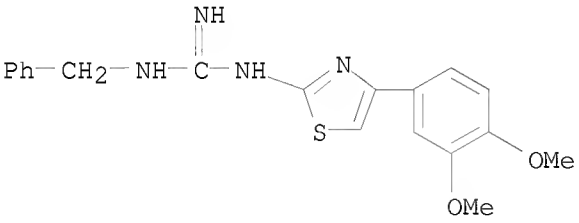

RN 123310-07-6 CAPLUS
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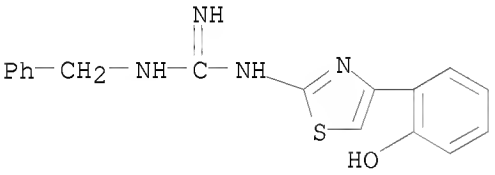
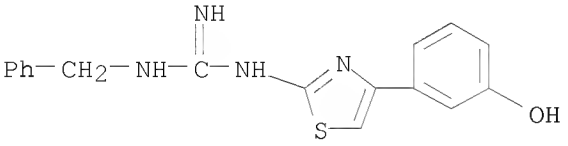
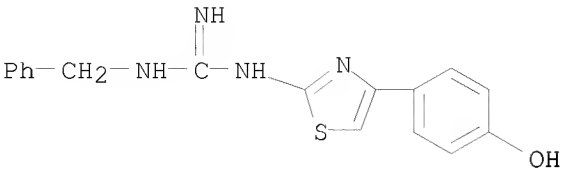


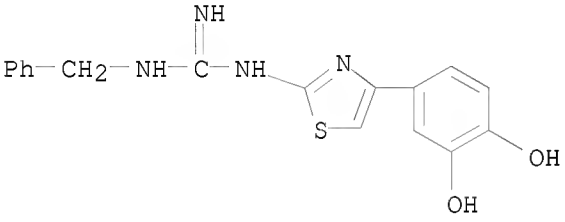
RN 123310-08-7 CAPLUS
CN Guanidine, N-[4-(3-hydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



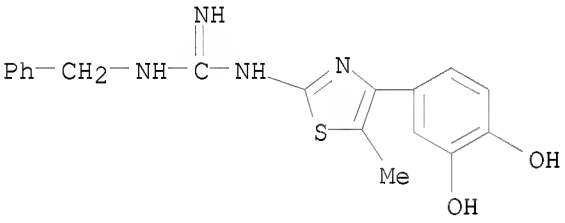
RN 123310-09-8 CAPLUS
CN Guanidine, N-[4-(4-hydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-11-2 CAPLUS
CN Guanidine, N-[4-(3,4-dihydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-13-4 CAPLUS
CN Guanidine, N-[4-(3,4-dihydroxyphenyl)-5-methyl-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)

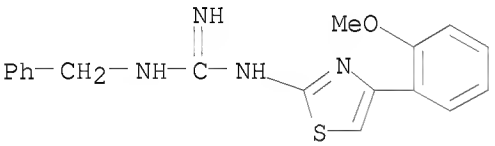


OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)

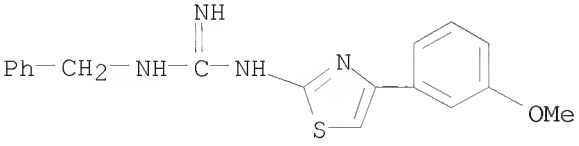
L6 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1994:94733 CAPLUS
DOCUMENT NUMBER: 120:94733
ORIGINAL REFERENCE NO.: 120:16615a,16618a
TITLE: Structure-activity relationship studies of 4-substituted-2-guanidinothiazoles: reversible inhibitors of gastric (hydrogen ion, potassium)-ATPase
AUTHOR(S): Ojha, T. N.; Singh, P.; Sharma, R. C.
CORPORATE SOURCE: Dep. Chem., S K Gov. Coll., Sikar, 332 001, India
SOURCE: Indian Journal of Biochemistry & Biophysics (1993), 30(4), 239-43
CODEN: IJBBBQ; ISSN: 0301-1208
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
The role of physicochem. factors, electronic and hydrophobic, and a hydrogen donor index in the inhibition of gastric (H+/K+)-ATPase by 4-phenyl-2-guanidinothiazoles and the 4-indolyl-2-guanidinothiazoles has been quant. analyzed. For the first congeneric series, the resonance effect of the ortho- and para-substituents and hydrogen donor property of the meta-substituent in the Ph ring play crucial role, whereas for 4-indolyl analogs, the hydrophobicity and electron withdrawing effect of X-substituents in the indolyl ring are shown to be important decisive factors. Also the substitution of the guanidine moiety, e.g. by benzyl, raises the activity of proton pump inhibitors. The substitution at 5-position of thiazole ring does not enhance the potency.

IT **123309-99-9** **123310-00-9** **123310-07-6** **123310-11-2**
RL: BIOL (Biological study)
(ATPase of stomach inhibition by, QSAR of)

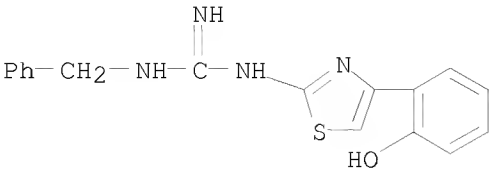
RN 123309-99-9 CAPLUS
CN Guanidine, N-[4-(2-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



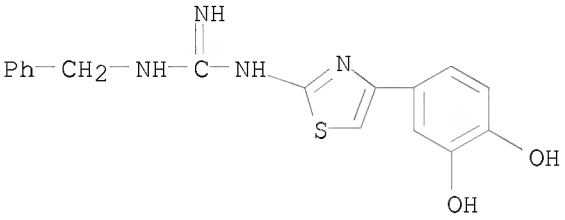
RN 123310-00-9 CAPLUS
CN Guanidine, N-[4-(3-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



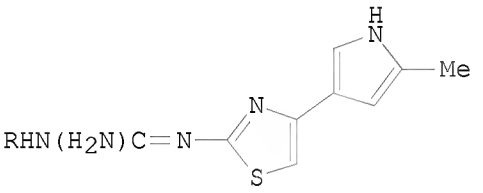
RN 123310-07-6 CAPLUS
CN Guanidine, N-[4-(2-hydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-11-2 CAPLUS
CN Guanidine, N-[4-(3,4-dihydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



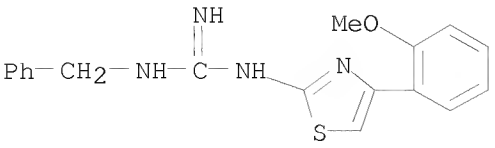
L6 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1990:55688 CAPLUS
DOCUMENT NUMBER: 112:55688
ORIGINAL REFERENCE NO.: 112:9563a,9566a
TITLE: Antiulcer agents. 4-Substituted 2-guanidinothiazoles: reversible, competitive, and selective inhibitors of gastric H+,K+-ATPase
AUTHOR(S): LaMattina, John L.; McCarthy, Peter A.; Reiter, Lawrence A.; Holt, William F.; Yeh, Li An
CORPORATE SOURCE: Cent. Res. Div., Pfizer Inc., Groton, CT, 06340, USA
SOURCE: Journal of Medicinal Chemistry (1990), 33(2), 543-52
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:55688
GRAPHIC IMAGE:



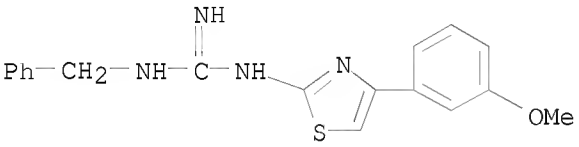
I

ABSTRACT:
A series of 4-substituted-2-guanidinothiazoles, e.g. (I, R = PhCH2, 4-ClC6H4CH2, hexyl), is shown to inhibit the gastric proton-pump enzyme, H+,K+-ATPase. In general, these compds. were reversible inhibitors of canine gastric H+,K+-ATPase, competitive at the K+-site, and selective relative to canine renal Na+,K+-ATPase. Structure-activity relationship (SAR) studies on this series revealed no general replacement for the guanidinothiazole. On the other hand, use of pyrrolyl, Ph, and indolyl groups as the C-4 substituent yielded active compds. Extensive studies of substitution patterns on these 4-aryl groups led to more active compds., but no consistent SAR became apparent. Monosubstitution of the guanidine and substitution of the thiazole at C-5 both often led to increased activity, but combining these changes generated compds. less active than the parents. Despite 100-fold improvement in in vitro inhibitory potency, only a 3-fold increase in gastric antisecretory activity in rats was observed for these agents.

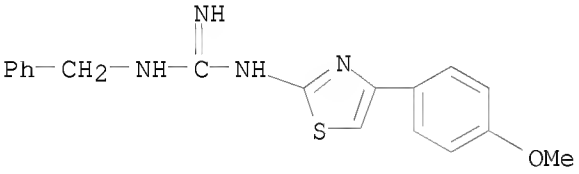
IT **123309-99-9P** **123310-00-9P** **123310-02-1P**
123310-04-3P **123310-07-6P** **123310-08-7P**
123310-09-8P **123310-11-2P** **123310-13-4P**
123310-82-7P **123310-83-8P** **123310-85-0P**
123310-87-2P **123310-89-4P** **123310-90-7P**
123310-91-8P **123310-93-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antiulcer activity of)
RN 123309-99-9 CAPLUS
CN Guanidine, N-[4-(2-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



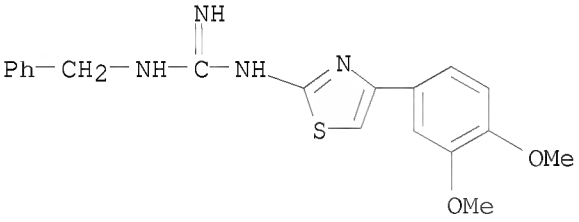
RN 123310-00-9 CAPLUS
CN Guanidine, N-[4-(3-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



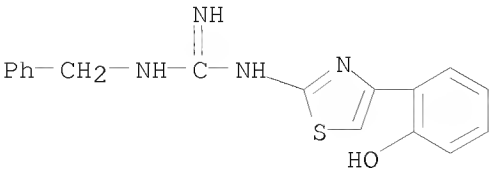
RN 123310-02-1 CAPLUS
CN Guanidine, N-[4-(4-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-04-3 CAPLUS
CN Guanidine, N-[4-(3,4-dimethoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



RN 123310-07-6 CAPLUS
CN Guanidine, N-[4-(2-hydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)- (CA INDEX NAME)



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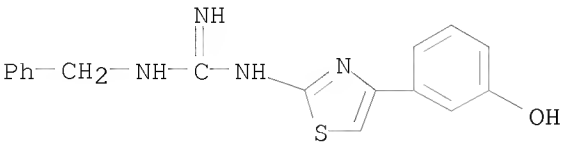

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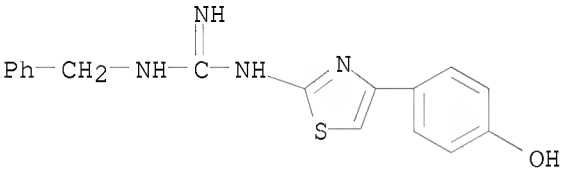

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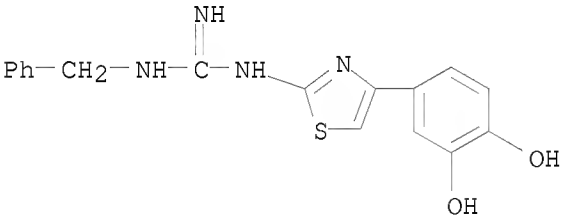

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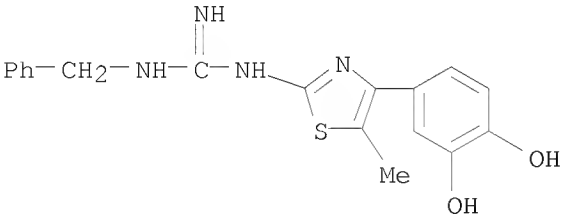
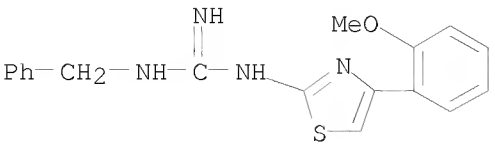


RN 123310-82-7 CAPLUS
CN Guanidine, N-[4-(2-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)-, hydrobromide (1:1) (CA INDEX NAME)



● HBr

RN 123310-83-8 CAPLUS
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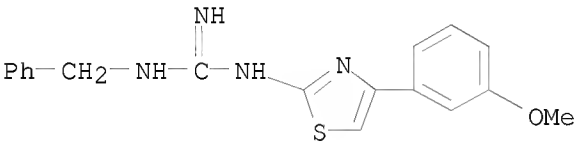
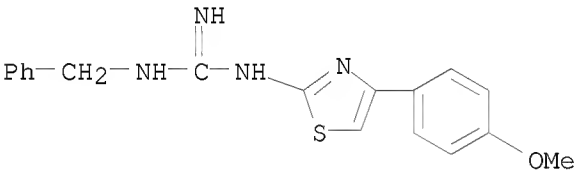


● HBr

RN 123310-85-0 CAPLUS
CN Guanidine, N-[4-(4-methoxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)-, hydrobromide (1:1) (CA INDEX NAME)



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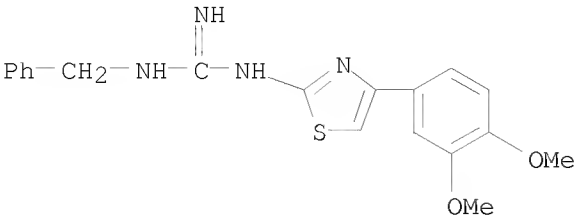

● HCl

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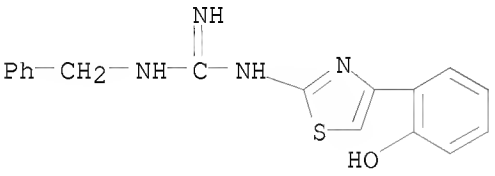

● HBr

RN 123310-90-7 CAPLUS
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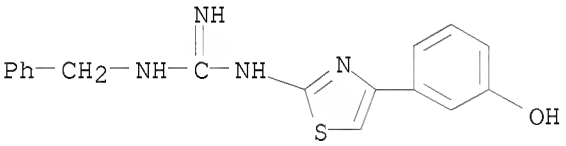

● HBr

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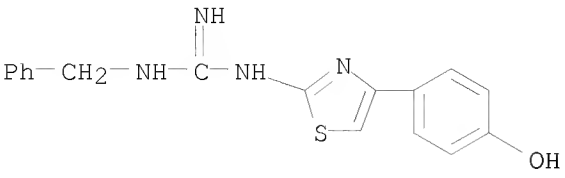

● HBr

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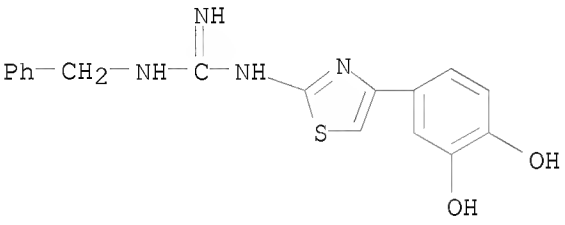
CN Guanidine, N-[4-(3,4-dihydroxyphenyl)-2-thiazolyl]-N'-(phenylmethyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

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L4          23 SEA ABB=ON  PLU=ON  L3 AND CAPLUS/LC
L5           2 SEA ABB=ON  PLU=ON  L3 NOT L4
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     DICTIONARY FILE UPDATES:  16 SEP 2011  HIGHEST RN 1332690-84-2

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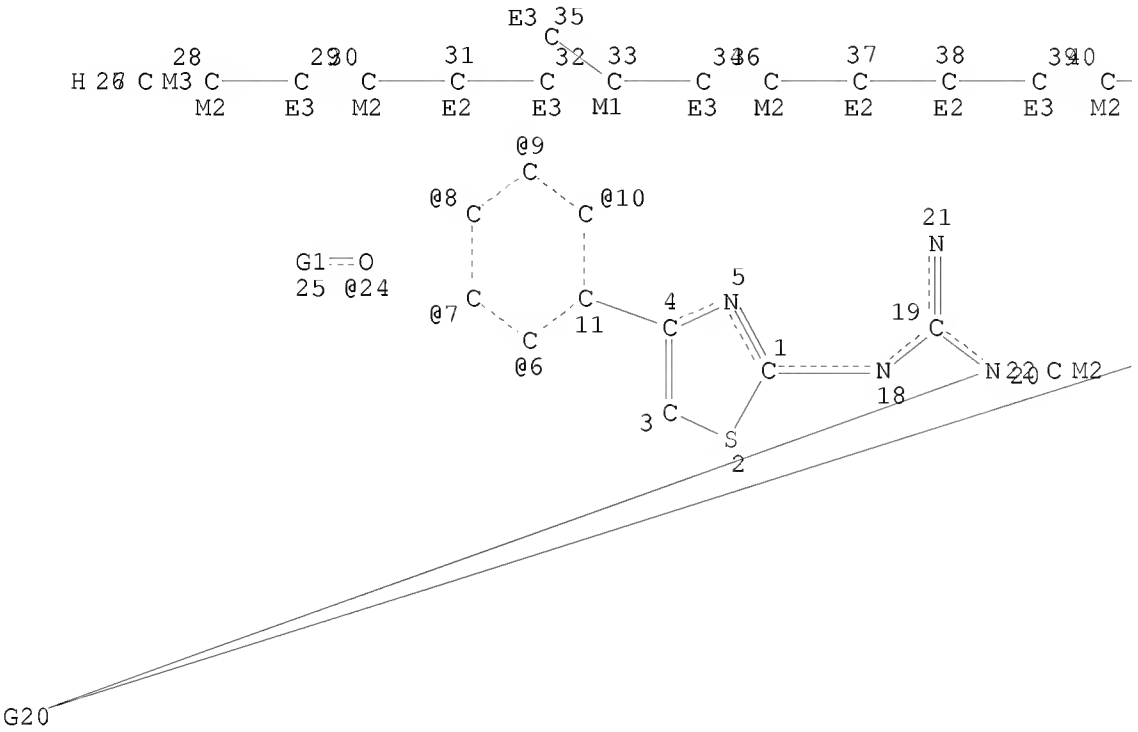

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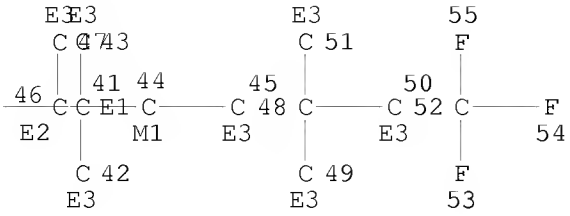

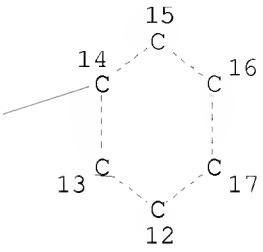

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Page 2-A
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